STIC Search Report
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STIC Database Tracking Number: 143802

TO: Shailendra Kumar **Location: 5c03 / 5c18** **Monday, February 07, 2005** **Art Unit: 1621** **Phone: 272-0640** **Serial Number: 10 / 769219**	**From: Jan Delaval** **Location: Biotech-Chem Library** **Rem 1a51** **Phone: 272-2504** **jan.delaval@uspto.gov**

Search Notes

Access DB# 143502

Jan please

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: S. Kumar Examiner #: 69594 Date: 1/31/05

Art Unit: 1621 Phone Number: 2-0640 Serial Number: 10/769,219

Mail Box and Bldg/Room Location: REM 5C03 5C18 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of invention: Beta 2-adrenergic agonists

Inventors (please provide full names): Edmund Moran et al.

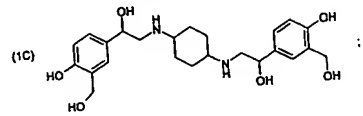
Earliest Priority Filing Date: 6/7/1999

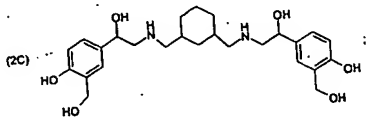
For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

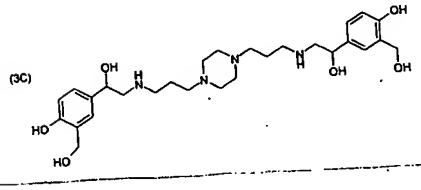
II. AMENDMENTS TO THE CLAIMS

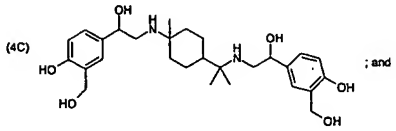
Please cancel Claims 1-49 without prejudice and insert new Claims 50-59.

50. A compound selected from the group consisting of:









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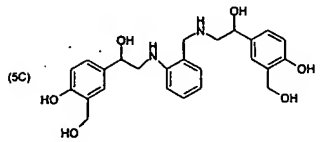

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Searcher Phone #: 22504

Searcher Location:

Date Searcher Picked Up: 2/7/05

Date Completed: 2/7/05

Searcher Prep & Review Time:

Clerical Prep Time: 15

Online Time: 15

Type of Search

NA Sequence (#)

AA Sequence (#)

Structure (#) ✓

Bibliographic

Litigation

Fulltext

Patent Family

Other

Vendors and cost where applicable

STN ✓

Dialog

Questel/Orbit

Dr.Link

Lexis/Nexis

Sequence Systems

WWW/Internet

Other (specify)

PTO-1590 (8-01)

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STRUCTURE FILE UPDATES:    6 FEB 2005  HIGHEST RN 826990-02-7
DICTIONARY FILE UPDATES:   6 FEB 2005  HIGHEST RN 826990-02-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
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Experimental and calculated property data are now available. For more
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http://www.cas.org/ONLINE/DBSS/registryss.html

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RL.P   Roles from patents:  BIOL (Biological study); PREP (Preparation); USES
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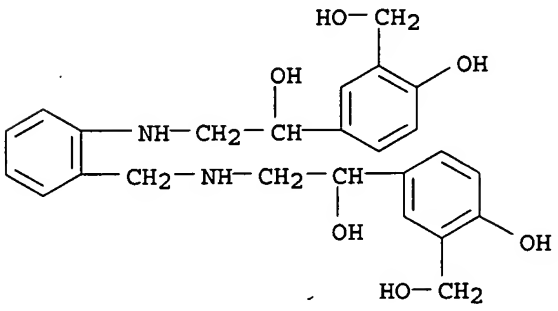


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REFERENCE   2:  135:45979
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REFERENCE 3: 134:131310

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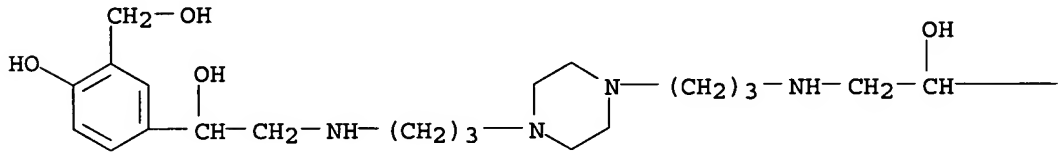

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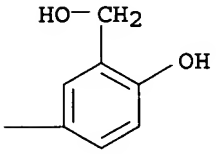

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L18 ANSWER 3 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
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MF C28 H42 N2 O6
SR CA
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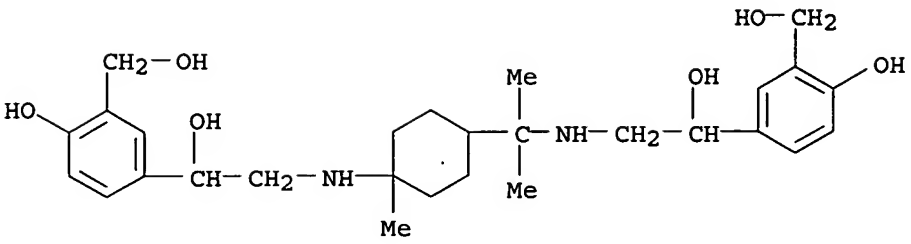

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REFERENCE 2: 135:45979

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L18 ANSWER 4 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
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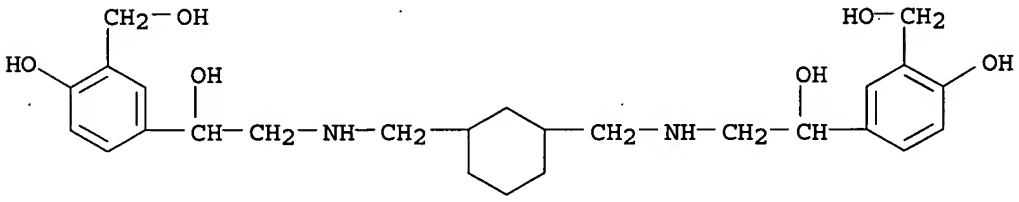

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L18 ANSWER 5 OF 5 REGISTRY COPYRIGHT 2005 ACS on STN
RN **321708-20-7** REGISTRY
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FS STEREOSEARCH

MF C24 H34 N2 O6
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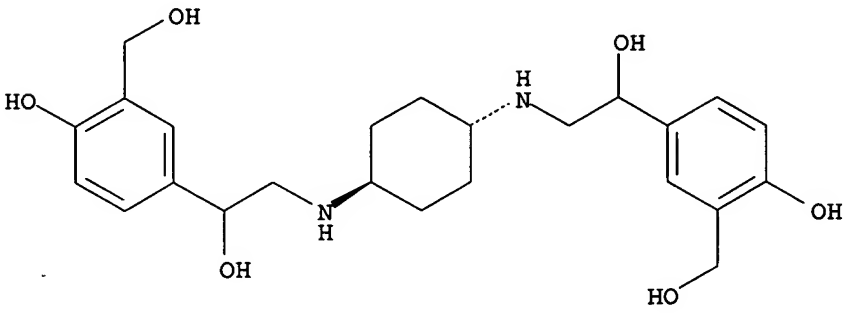
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Relative stereochemistry.



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E CHOI S/AU
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FILE COVERS 1907 - 7 Feb 2005  VOL 142 ISS 7
FILE LAST UPDATED: 6 Feb 2005  (20050206/ED)

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 substance identification.


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L21  ANSWER 1 OF 3  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2002:354101  HCAPLUS
DN   136:355062
ED   Entered STN:  12 May 2002
TI   Preparation of novel multi-binding phenolic compounds as
     β2-adrenergic receptor agonists
IN   Moran, Edmund J.; Griffin, John H.; Choi, Seok-ki
PA   Theravance, Inc., USA
SO   U.S. Pat. Appl. Publ., 92 pp., Cont. of U.S. Ser. No. 323,943.
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LA   English
IC   ICM  C07F009-22
     ICS  C07C311-15; C07C235-32; C07C215-28
NCL  564355000
CC   25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
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Section cross-reference(s): 1, 63

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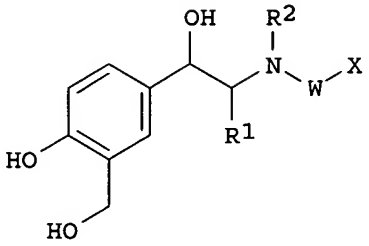
US 2003087306	ECLA	C07B061/00L; C07D263/32; C07D263/34D; C07D265/32; C07D277/24; C07D277/28; C07D277/34; C07D; C07D401/14R+257+211; C07D401/14R+249B+211; C07D413/06+265D+249B; C07D413/14R+265D+29B; C07D417/12+277B+263B; C07D417/12+277B+213; C07K001/04C; G01N033/94B; C07C215/60; C07C323/62; C07D211/42; C07D211/56; C07D213/74D6; C07D213/80B3 <--
US 2003087307	ECLA	A61K031/137; C07C215/68; C07C233/43; A61K031/167; C07C215/60

OS MARPAT 136:355062

GI



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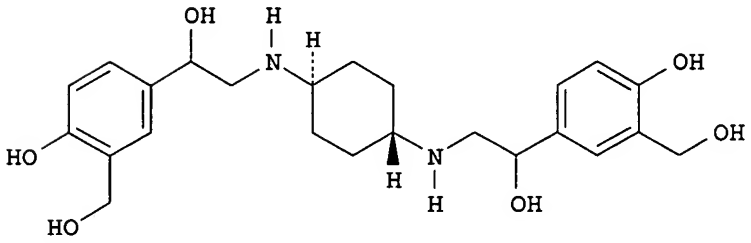


II

AB Methods for preparing novel multibinding phenolic compds., LpXq [where L = a ligand capable of binding to a β2-adrenergic receptor; X = a linker; p = 2-10; q = 1-20], which serve as β2-adrenergic receptor agonists, are disclosed. Preferred ligands are of formula I [R1 = H, (un)substituted alkyl, or a bond linking ligand to linker; R2 = H, aralkyl, acyl, (un)substituted alkyl, cycloalkyl or a bond linking ligand to linker; W = bond, (un)substituted alkylene wherein one or more carbon atoms is optionally replaced by NR3, O, S, SO, SO2, CO, P-alkyl, PO2, OP(O)O or the alkylene optionally links the ligand to a linker with provisions; R3 = H, alkyl, acyl, or bond linking ligand to linker; X = aryl, heteroaryl, heterocyclyl and (un)substituted cycloalkyl wherein each

X optionally links the ligand to the linker]. II was prepared from α,α-dihydroxy-4-hydroxy-3-methoxycarbonylacetophenone via condensation with trans-1,4-diaminocyclohexane with subsequent reduction of intermediate imine. In addition, combinatorial arrays of multimeric ligands and methods of assaying the multimeric ligands are embodied by the invention. As β2-adrenergic receptor agonists, the compds. are useful in the treatment and prevention of respiratory diseases such as asthma, bronchitis (no data). The title compds. are also useful in the treatment of nervous system injuries and premature labor. Formulations for capsules, tablets, dry power inhaler, suppositories and suspensions are described.

ST phenol multibinding prepn beta adrenergic receptor agonist; combinatorial array multibinding phenol beta adrenergic receptor agonist; multimeric ligand beta adrenergic receptor agonist; adrenergic receptor agonist respiratory disease prevention asthma bronchitis

IT Structure-activity relationship
(ligand-binding; preparation of phenolic β2-adrenergic receptor agonists)

IT Antiasthmatics
Combinatorial library
Drug delivery systems
(preparation of phenolic β2-adrenergic receptor agonists)

IT Respiratory tract, disease
(treatment of; preparation of phenolic β2-adrenergic receptor agonists)

IT Adrenoceptor agonists
(β2-; preparation of phenolic β2-adrenergic receptor agonists)

IT Adrenoceptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(β2; preparation of phenolic β2-adrenergic receptor agonists)

IT **321708-20-7P**, 1,3-Benzenedimethanol, α1,α1'-[trans-1,4-cyclohexanediylbis(iminomethylene)]bis[4-hydroxy- 321708-23-0P, 1,3-Benzenedimethanol, α1,α1'-[methylenebis(4,1-cyclohexanediyliminomethylene)]bis[4-hydroxy- **321708-25-2P**, 1,3-Benzenedimethanol, α1,α1'-[1,3-cyclohexanediylbis(methyleneiminomethylene)]bis[4-hydroxy- **321708-27-4P**, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[1-[4-[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]-4-methylcyclohexyl]-1-methylethyl]amino]methyl]- **321708-29-6P**, 1,3-Benzenedimethanol, α1,α1'-[1,4-piperazinediylbis(3,1-propanediyliminomethylene)]bis[4-hydroxy- 321708-31-0P, 1,3-Benzenedimethanol, α1,α1'-[1,4-phenylenebis(methyleneiminomethylene)]bis[4-hydroxy- 321708-33-2P, 1,3-Benzenedimethanol, α1,α1'-[1,3-phenylenebis(methyleneiminomethylene)]bis[4-hydroxy- **321708-35-4P**, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[2-[[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]methyl]phenyl]amino]methyl]- 321708-37-6P, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[4-[2-[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]ethyl]phenyl]amino]methyl]- 321708-39-8P, 1,3-Benzenedimethanol, α1,α1'-[oxybis(4,1-phenyleneiminomethylene)]bis[4-hydroxy- 321708-41-2P, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[4-[[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]methyl]phenyl]amino]methyl]- 321708-43-4P, 1,3-Benzenedimethanol, 4-hydroxy-α-[[[2-[4-[(2-hydroxy-2-phenylethyl)amino]phenyl]ethyl]amino]methyl]- 321708-45-6P, Benzenemethanol, α-[[[4-[2-[(2-hydroxy-2-phenylethyl)amino]ethyl]phenyl]amino]methyl]- 321708-47-8P, 1,3-Benzenedimethanol, 4-hydroxy-α-[[[2-[4-[(2-hydroxy-2-phenylethyl)amino]phenyl]ethyl]amino]methyl]-, mono(trifluoroacetate) (salt) 321708-49-0P, 1,3-Benzenedimethanol, 4-hydroxy-α-[[[2-[4-[[(2S)-2-hydroxy-2-phenylethyl]amino]phenyl]ethyl]amino]methyl]- 321708-51-4P, 1,3-Benzenedimethanol, 4-hydroxy-α-[[[2-[4-[[(2R)-2-hydroxy-2-phenylethyl]amino]phenyl]ethyl]amino]methyl]- 321708-53-6P, 1,3-Benzenedimethanol, α1,α1'-[1,6-hexanediylbis(oxy-4,1-

phenylene-3,1-propanediyloxy-6,1-hexanediyliminomethylene)]bis[4-hydroxy-
321708-54-7P, 1,3-Benzenedimethanol, 4-hydroxy-α-[[[2-[4-[[(2S)-2-
hydroxy-2-phenylethyl]amino]phenyl]ethyl]amino]methyl]-, (αR)-
321708-56-9P, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[6-[3-[4-[[6-[[2-
hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]hexyl]oxy]phenyl]
propoxy]hexyl]amino]methyl]- 321708-57-0P, 1,3-Benzenedimethanol,
α1,α1'-[1,3-phenylenebis[oxy(2-hydroxy-3,1-
propanediyl)iminomethylene]]bis[4-hydroxy- 321708-60-5P,
1,3-Benzenedimethanol, 4-hydroxy-α-[[[2-[4-[[2-hydroxy-3-(1-
naphthalenyloxy)propyl]amino]phenyl]ethyl]amino]methyl]- 321709-02-8P,
1,3-Benzenedimethanol, α1,α1'-[[4-[[[2-hydroxy-2-[4-hydroxy-3-
(hydroxymethyl)phenyl]ethyl]amino]methyl]-1,8-
octanediyl]bis(iminomethylene)]bis[4-hydroxy-
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
(preparation of phenolic β2-adrenergic receptor agonists)

IT 80-52-4, 1,8-Diamino-p-menthane 100-39-0, Benzylbromide 100-52-7,
Benzaldehyde, reactions 101-80-4, 4,4'-Oxydianiline 101-90-6,
Resorcinol diglycidyl ether 539-48-0, 1,4-Benzenedimethanamine
629-09-4, 1,6-Diiodohexane 1075-06-5, α,α-
Dihydroxyacetophenone 1477-55-0, 1,3-Benzenedimethanamine 1572-55-0,
1,8-Octanediamine, 4-(aminomethyl)- 1761-71-3, 4,4'-
Methylenebis(cyclohexylamine) 2461-42-9, Oxirane, [(1-
naphthalenyloxy)methyl]- 2579-20-6, 1,3-Cyclohexanebis(methylamine)
2615-25-0, trans-1,4-Diaminocyclohexane 4403-69-4, 2-Aminobenzylamine
4403-71-8, 4-Aminobenzylamine 6621-59-6, 6-Bromohexanenitrile
7209-38-3, 1,4-Bis(3-aminopropyl)piperazine 10210-17-0,
3-(4-Hydroxyphenyl)-1-propanol 13472-00-9, 2-(4-Aminophenyl)ethylamine
16475-90-4, Benzoic acid, 5-acetyl-2-hydroxy-, methyl ester 20780-53-4,
Oxirane, phenyl-, (2R)- 94749-70-9, Benzoic acid, 5-(2R)-oxiranyl-2-
(phenylmethoxy)-, methyl ester 321709-19-7, Benzenemethanol,
α-[[[4-(2-aminoethyl)phenyl]amino]methyl]-, (αR)-
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenolic β2-adrenergic receptor agonists)

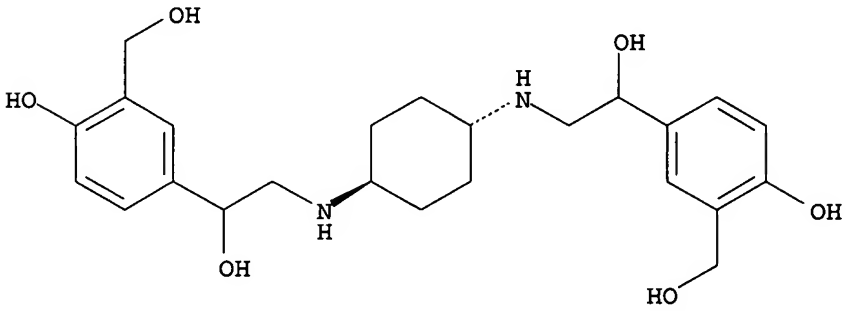
IT 27475-09-8P, Benzoic acid, 5-acetyl-2-(phenylmethoxy)-, methyl ester
27475-14-5P, Benzoic acid, 5-(bromoacetyl)-2-(phenylmethoxy)-, methyl
ester 29754-58-3P, Benzoic acid, 5-(dihydroxyacetyl)-2-hydroxy-, methyl
ester 92900-77-1P, 1,3-Benzenedimethanol, α1-(aminomethyl)-4-
(phenylmethoxy)- 94838-59-2P, Carbamic acid, [2-(4-aminophenyl)ethyl]-,
1,1-dimethylethyl ester 321708-64-9P, Carbamic acid,
[2-[4-[(2-hydroxy-2-phenylethyl)amino]phenyl]ethyl]-, 1,1-dimethylethyl
ester 321708-67-2P, Benzenemethanol, α-[[[4-(2-
aminoethyl)phenyl]amino]methyl]-, mono(trifluoroacetate) (salt)
321708-69-4P, Carbamic acid, [2-[4-[[(2S)-2-hydroxy-2-
phenylethyl]amino]phenyl]ethyl]-, 1,1-dimethylethyl ester 321708-72-9P,
Benzenemethanol, α-[[[4-(2-aminoethyl)phenyl]amino]methyl]-,
(αS)-, mono(trifluoroacetate) (salt) 321708-74-1P,
Benzenepropanol, 4,4'-[1,6-hexanediylbis(oxy)]bis- 321708-76-3P,
Hexanenitrile, 6,6'-[1,6-hexanediylbis(oxy-4,1-phenylene-3,1-
propanediyloxy)]bis- 321708-78-5P, Hexanoic acid, 6,6'-[1,6-
hexanediylbis(oxy-4,1-phenylene-3,1-propanediyloxy)]bis- 321708-80-9P,
1,3-Benzenedimethanol, α1,α1'-[1,6-hexanediylbis(oxy-4,1-
phenylene-3,1-propanediyloxy-6-hexanyl-1-ylidenenitrilomethylene)]bis[4-
(phenylmethoxy)- 321708-82-1P, Carbamic acid, [2-[4-
[(phenylmethyl)amino]phenyl]ethyl]-, 1,1-dimethylethyl ester
321708-84-3P, Carbamic acid, [2-[4-[[(2S)-2-hydroxy-2-
phenylethyl](phenylmethyl)amino]phenyl]ethyl]-, 1,1-dimethylethyl ester
321708-86-5P, Benzenemethanol, α-[[[4-(2-
aminoethyl)phenyl](phenylmethyl)amino]methyl]-, (αS)-
321708-88-7P, Benzenemethanol, α-[[(phenylmethyl)[4-[2-
[(phenylmethyl)amino]ethyl]phenyl]amino]methyl]-, (αS)-
321708-89-8P, Benzoic acid, 5-[(1R)-1-hydroxy-2-[[2-[4-[[(2S)-2-hydroxy-2-

phenylethyl](phenylmethyl)amino]phenyl]ethyl](phenylmethyl)amino]ethyl]-2-(phenylmethoxy)-, methyl ester 321708-90-1P, 1,3-Benzenedimethanol, α-[[[2-[4-[[(2S)-2-hydroxy-2-phenylethyl](phenylmethyl)amino]phenyl]ethyl](phenylmethyl)amino]methyl]-4-(phenylmethoxy)-, (αR)- 321708-92-3P, Hexanenitrile, 6-[3-[4-[(5-cyanopentyl)oxy]phenyl]propoxy]- 321708-94-5P, 1-Hexanamine, 6-[4-[3-[(6-aminohexyl)oxy]propyl]phenoxy]- 321708-98-9P, Benzoic acid, 5-(azidoacetyl)-2-(phenylmethoxy)-, methyl ester 321709-00-6P, Carbamic acid, [2-[4-[[2-hydroxy-3-(1-naphthalenyloxy)propyl]amino]phenyl]ethyl]-, 1,1-dimethylethyl ester 321710-07-0P, 1,3-Benzenedimethanol, α1,α1'-[1,6-hexanediylbis(oxy-4,1-phenylene-3,1-propanediyloxy-6,1-hexanediyliminomethylene)]bis[4-(phenylmethoxy)-
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenolic β2-adrenergic receptor agonists)

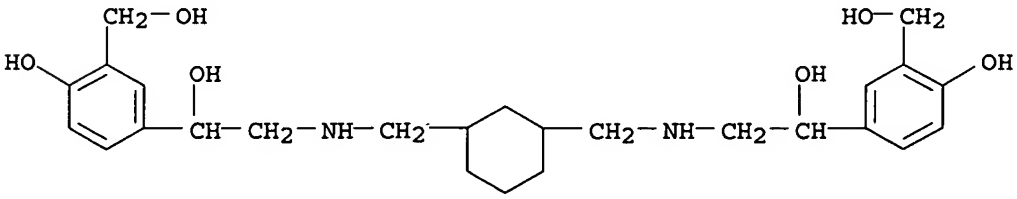
IT **321708-20-7P**, 1,3-Benzenedimethanol, α1,α1'-[trans-1,4-cyclohexanediylbis(iminomethylene)]bis[4-hydroxy- **321708-25-2P**, 1,3-Benzenedimethanol, α1,α1'-[1,3-cyclohexanediylbis(methyleneiminomethylene)]bis[4-hydroxy- **321708-27-4P**, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[1-[4-[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]-4-methylcyclohexyl]-1-methylethyl]amino]methyl]- **321708-29-6P**, 1,3-Benzenedimethanol, α1,α1'-[1,4-piperazinediylbis(3,1-propanediyliminomethylene)]bis[4-hydroxy- **321708-35-4P**, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[2-[[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]methyl]phenyl]amino]methyl]-
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenolic β2-adrenergic receptor agonists)

RN 321708-20-7 HCAPLUS
CN 1,3-Benzenedimethanol, α1,α1'-[trans-1,4-cyclohexanediylbis(iminomethylene)]bis[4-hydroxy- (9CI) (CA INDEX NAME)

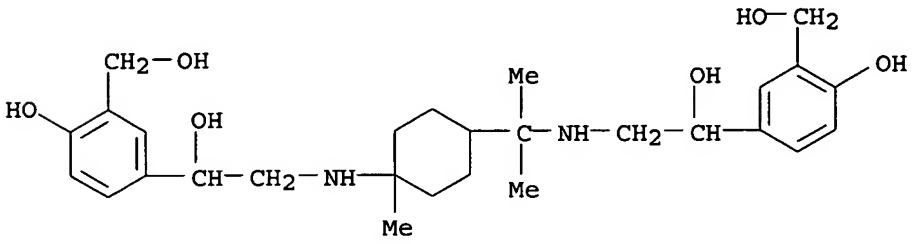
Relative stereochemistry.



RN 321708-25-2 HCAPLUS
CN 1,3-Benzenedimethanol, α1,α1'-[1,3-cyclohexanediylbis(methyleneiminomethylene)]bis[4-hydroxy- (9CI) (CA INDEX NAME)

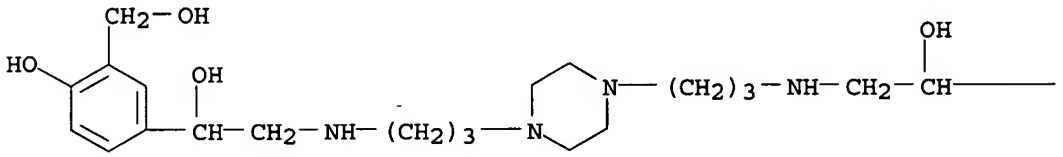


RN 321708-27-4 HCAPLUS
CN 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[1-[4-[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]-4-methylcyclohexyl]-1-methylethyl]amino]methyl]- (9CI) (CA INDEX NAME)

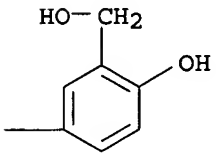


RN 321708-29-6 HCAPLUS
CN 1,3-Benzenedimethanol, α1,α1'-[1,4-piperazinediylbis(3,1-propanediyliminomethylene)]bis[4-hydroxy- (9CI) (CA INDEX NAME)

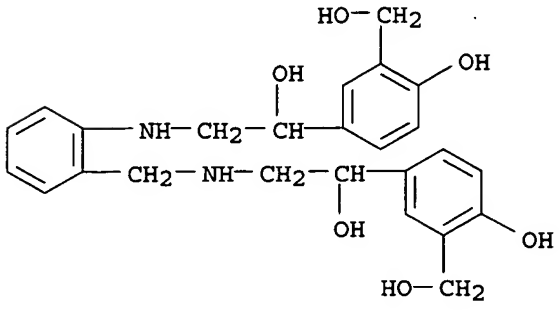
PAGE 1-A



PAGE 1-B



RN 321708-35-4 HCAPLUS
CN 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[2-[[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]methyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)



L21 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:435027 HCAPLUS
DN 135:45979
ED Entered STN: 15 Jun 2001
TI Preparation of 4-(arylhydroxyethylaminoethyl)phenylaminohydroxyethylbenzenes and related compounds as β2 adrenergic receptor agonists and partial agonists.
IN **Moran, Edmund J.**; Griffin, John H.; **Choi, Seok-ki**
PA Advanced Medicine, Inc., USA
SO PCT Int. Appl., 164 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07C233-43
ICS C07C215-68; A61K031-135; A61K031-165; A61P011-00; A61P025-00
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 27
FAN.CNT 31

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PI	WO 2001042193	A1	20010614	WO 2000-US33057	20001206
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	BR 2000015962	A	20020730	BR 2000-15962	20001206
	EP 1235787	A1	20020904	EP 2000-986271	20001206
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	PT 1235787	T	20040331	PT 2000-986271	20001206
	ES 2208453	T3	20040616	ES 2000-986271	20001206
	US 2003087307	A1	20030508	US 2002-108945	20020328
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	HK 1048803	A1	20040130	HK 2003-101047	20030213
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	US 2000-637899	A1	20000814		
	US 1999-323943	A2	19990602		
	WO 2000-US33057	W	20001206		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001042193	ICM	C07C233-43
	ICS	C07C215-68; A61K031-135; A61K031-165; A61P011-00; A61P025-00
US 2003087307	ECLA	A61K031/137; C07C215/68; C07C233/43; A61K031/167; C07C215/60

AB LpXq [p= 2-10; q = 1-20; X = linker, L = ligand; 1 ligand = Ar1CH(OH)CHR1NR2WAr2, the other = QAr3; Ar1, Ar2 = aryl, heteroaryl, heterocyclyl, (substituted) cycloalkyl; R1 = H, (substituted) alkyl, bond to linker; R2 = H, aralkyl, acyl, (substituted) alkyl, cycloalkyl, bond to linker; W = bond, (substituted) (heteroatom-interrupted) alkylene; Ar3 =

aryl, heteroaryl, (substituted) cycloalkyl, heterocyclyl; Q = bond, (substituted) (heteroatom-interrupted) alkylene; with provisos], were prepared for treatment of respiratory diseases (no data). Thus, α,α-hydroxy-4-hydroxy-3-methoxycarbonylacetophenone (preparation given) was stirred with trans-1,4-diaminocyclohexane in THF for 3 h at room temperature followed by addition of BH3/Me2S in hexane and stirring for 4 h to give trans-1,4-bis[N-[2-(4-hydroxy-3-hydroxymethylphenyl)-2-hydroxyethyl]amino]cyclohexane.

ST arylhydroxyethylaminoethylphenylaminohydroxyethylbenzene prepn adrenergic agonist; chronic obstructive pulmonary disease treatment arylhydroxyethylaminoethylphenylaminohydroxyethylbenzene prepn; antiasthmatic arylhydroxyethylaminoethylphenylaminohydroxyethylbenzene prepn

IT Lung, disease
(chronic obstructive, treatment; preparation of arylhydroxyethylaminoethylphenylaminohydroxyethylbenzenes and related compds. as β2 adrenergic receptor agonists and partial agonists)

IT Antiasthmatics
(preparation of arylhydroxyethylaminoethylphenylaminohydroxyethylbenzenes and related compds. as β2 adrenergic receptor agonists and partial agonists)

IT Adrenoceptor agonists
(β2-; preparation of arylhydroxyethylaminoethylphenylaminohydroxyethylbenzenes and related compds. as β2 adrenergic receptor agonists and partial agonists)

IT **321708-20-7P** 321708-23-0P **321708-25-2P**
321708-27-4P **321708-29-6P** 321708-31-0P 321708-33-2P
321708-35-4P 321708-37-6P 321708-39-8P 321708-41-2P
321708-43-4P 321708-45-6P 321708-47-8P 321708-49-0P 321708-51-4P
321708-53-6P 321708-56-9P 321708-57-0P 321708-60-5P 321709-02-8P
344466-40-6P 344466-41-7P 344466-42-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylhydroxyethylaminoethylphenylaminohydroxyethylbenzenes and related compds. as β2 adrenergic receptor agonists and partial agonists)

IT 70-11-1, α-Bromoacetophenone 80-52-4 100-52-7, Benzaldehyde, reactions 101-80-4 101-90-6, Resorcinol diglycidyl ether 107-22-2, Glyoxal 539-48-0, p-Xylylenediamine 629-09-4, 1,6-Diiodohexane 1074-12-0, Phenylglyoxal 1075-06-5, α,α-Dihydroxyacetophenone 1477-55-0, 1,3-Benzenedimethanamine 1572-55-0, 4-Aminomethyl-1,8-octanediamine 1761-71-3 2461-42-9 2579-20-6, 1,3-Cyclohexanedimethanamine 2615-25-0, trans-1,4-Diaminocyclohexane 4403-69-4, 2-Aminobenzylamine 4403-71-8, 4-Aminobenzylamine 6621-59-6, 6-Bromohexanenitrile 7209-38-3, 1,4-Piperazinedipropanamine 10210-17-0, 3-(4-Hydroxyphenyl)-1-propanol 13472-00-9, 2-(4-Aminophenyl)ethylamine 16475-90-4, Methyl 5-acetylsalicylate 20780-53-4 37148-47-3 43229-01-2 94749-70-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylhydroxyethylaminoethylphenylaminohydroxyethylbenzenes and related compds. as β2 adrenergic receptor agonists and partial agonists)

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(preparation of arylhydroxyethylaminoethylphenylaminohydroxyethylbenzenes and related compds. as β2 adrenergic receptor agonists and partial agonists)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Advanced Medicine Inc; WO 9964035 A 1999 HCAPLUS
(2) Anon; PATENT ABSTRACTS OF JAPAN 1998, V1998(11)
(3) Degussa; GB 1040724 A 1966
(4) Kissei Pharmaceut Co Ltd; JP 10152460 A 1998 HCAPLUS
(5) Sepracor Inc; WO 9821175 A 1998 HCAPLUS
(6) Thomae Gmbh Dr K; GB 1394542 A 1975 HCAPLUS

IT **321708-20-7P 321708-25-2P 321708-27-4P**
321708-29-6P 321708-35-4P
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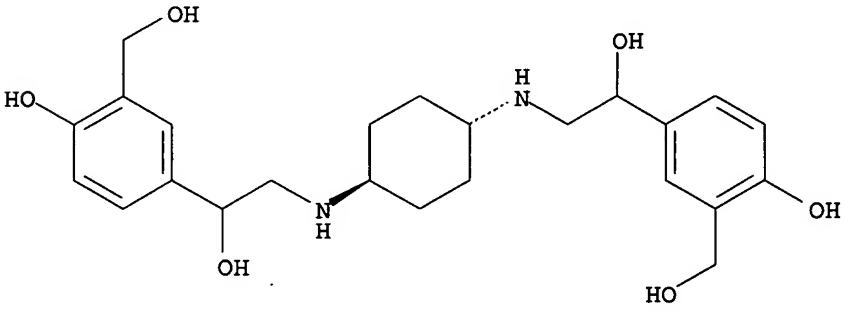
Relative stereochemistry.



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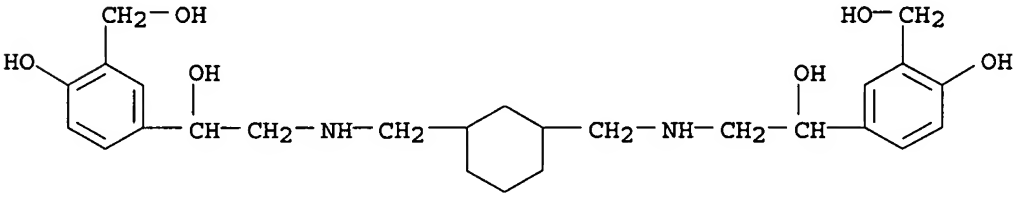

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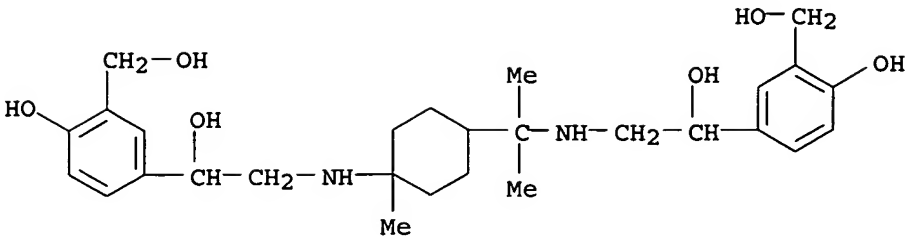

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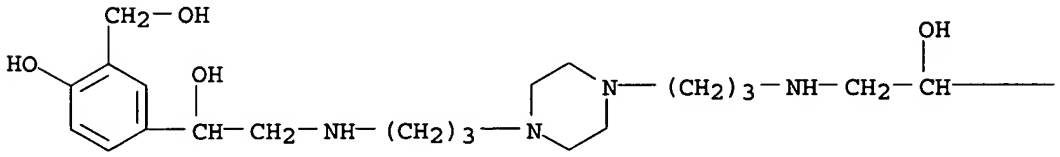

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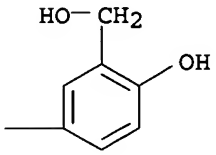

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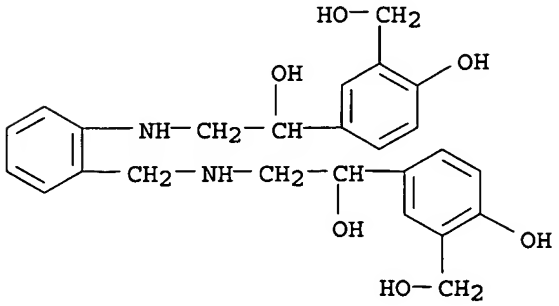

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TI Preparation of novel multibinding phenolic compounds as β2-adrenergic receptor agonists

IN Griffin, John H.; **Moran, Edmund J.**; **Choi, Seok-Ki**
PA Advanced Medicine, Inc., USA
SO PCT Int. Appl., 159 pp.
CODEN: PIXXD2
DT Patent
LA English
IC A61K038-00; A61K039-00; A61K039-44; A61K039-395; A61K051-00; G01N033-53; G01N033-543; G01N033-566; C07C213-00
CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 63
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CLASS

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C07D413/06+265D+249B; C07D413/14R+265D+249B;
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C07D413/06+265D+249B; C07D413/14R+265D+249B;
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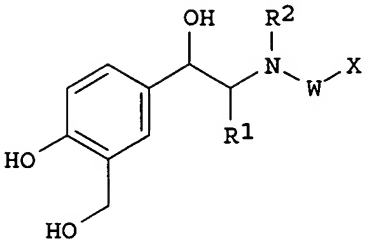

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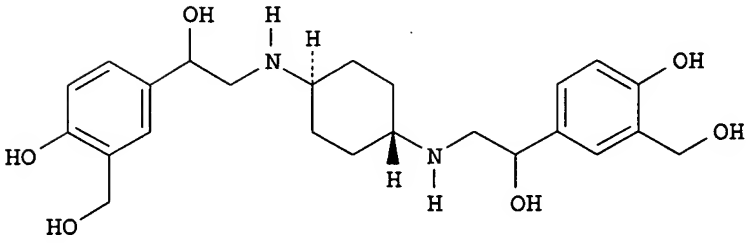

II

AB Methods for preparing novel multibinding phenolic compds., LpXq [where L = a ligand capable of binding to a β2-adrenergic receptor; X = a linker; p = 2-10; q = 1-20], which serve as β2-adrenergic receptor agonists, are disclosed. Preferred ligands are of formula I [R1 = H, (un)substituted alkyl, or a bond linking ligand to linker; R2 = H, aralkyl, acyl, (un)substituted alkyl, cycloalkyl or a bond linking ligand to linker; W = bond, (un)substituted alkylene wherein one or more carbon atoms is optionally replaced by NR3, O, S, SO, SO2, CO, P-alkyl, PO2, OP(O)O or the alkylene optionally links the ligand to a linker with provisions; R3 = H, alkyl, acyl, or bond linking ligand to linker; X = aryl, heteroaryl, heterocyclyl and (un)substituted cycloalkyl wherein each X optionally links the ligand to the linker]. II was prepared from α,α-dihydroxy-4-hydroxy-3-methoxycarbonylacetophenone via condensation with trans-1,4-diaminocyclohexane with subsequent reduction of intermediate imine. In addition, combinatorial arrays of multimeric ligands and methods of assaying the multimeric ligands are embodied by the invention. As β2-adrenergic receptor agonists, the compds. are useful in the treatment and prevention of respiratory diseases such as asthma, bronchitis (no data). The title compds. are also useful in the treatment of nervous system injuries and premature labor. Formulations for capsules, tablets, dry power inhaler, suppositories and suspensions are described.

ST phenol multibinding prepn beta adrenergic receptor agonist; combinatorial

array multibinding phenol beta adrenergic receptor agonist; multimeric ligand beta adrenergic receptor agonist; adrenergic receptor agonist respiratory disease prevention asthma bronchitis

IT Respiratory tract
(disease, treatment of; preparation of phenolic β2-adrenergic receptor agonists)

IT Structure-activity relationship
(ligand-binding; preparation of phenolic β2-adrenergic receptor agonists)

IT Antiasthmatics
Combinatorial library
Drug delivery systems
(preparation of phenolic β2-adrenergic receptor agonists)

IT Adrenoceptor agonists
(β2-; preparation of phenolic β2-adrenergic receptor agonists)

IT Adrenoceptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(β2; preparation of phenolic β2-adrenergic receptor agonists)

IT **321708-20-7P** 321708-23-0P **321708-25-2P**
321708-27-4P **321708-29-6P** 321708-31-0P 321708-33-2P
321708-35-4P 321708-37-6P 321708-39-8P 321708-41-2P
321708-43-4P 321708-45-6P 321708-47-8P 321708-49-0P 321708-51-4P
321708-53-6P 321708-54-7P 321708-56-9P 321708-57-0P 321708-60-5P
321709-02-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenolic β2-adrenergic receptor agonists)

IT 80-52-4, 1,8-Diamino-p-menthane 100-39-0, Benzylbromide 100-52-7, Benzaldehyde, reactions 101-80-4, 4,4'-Oxydianiline 101-90-6, Resorcinol diglycidyl ether 539-48-0, 1,4-Benzenedimethanamine 629-09-4, 1,6-Diiodohexane 1075-06-5, α,α-Dihydroxyacetophenone 1477-55-0, 1,3-Benzenedimethanamine 1572-55-0 1761-71-3, 4,4'-Methylenebis(cyclohexylamine) 2461-42-9 2579-20-6, 1,3-Cyclohexanebis(methylamine) 2615-25-0, trans-1,4-Diaminocyclohexane 4403-69-4, 2-Aminobenzylamine 4403-71-8, 4-Aminobenzylamine 6621-59-6, 6-Bromohexanenitrile 7209-38-3, 1,4-Bis(3-aminopropyl)piperazine 10210-17-0, 3-(4-Hydroxyphenyl)-1-propanol 13472-00-9, 2-(4-Aminophenyl)ethylamine 16475-90-4 20780-53-4 94749-70-9 321709-19-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenolic β2-adrenergic receptor agonists)

IT 27475-09-8P 27475-14-5P 29754-58-3P 92900-77-1P 94838-59-2P
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321708-76-3P 321708-78-5P 321708-80-9P 321708-82-1P 321708-84-3P
321708-86-5P 321708-88-7P 321708-89-8P 321708-90-1P 321708-92-3P
321708-94-5P 321708-98-9P 321709-00-6P 321710-07-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenolic β2-adrenergic receptor agonists)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Goodman; US 4587046 A 1986 HCAPLUS
(2) Janssen, P; A New Form of Cardiovascular Therapy? 1991, V3(Suppl 1), P1
(3) Kierstead; J Med Chem 1983, V26, P1561 HCAPLUS
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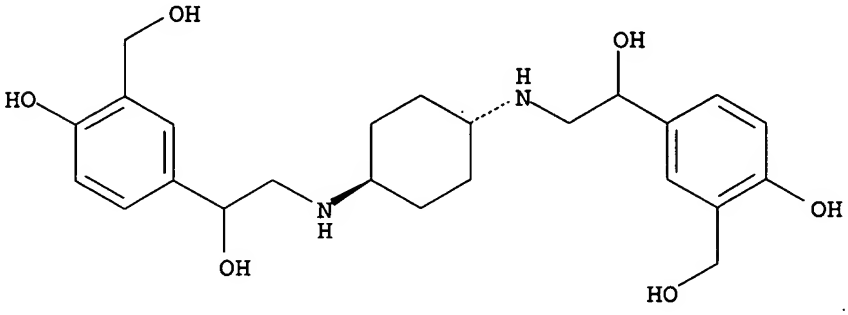
(6) Pitha; J Med Chem 1983, V26, P7 HCAPLUS
(7) Pitha; Proc Natl Acad Sci USA 1990, V77(4), P2219
(8) Shuker; Science 1996, V274, P1531 HCAPLUS
(9) Siegel; Mol Diversity 1998, V3(2), P113
(10) The Salk Institute For Biological Studies; WO 9735195 A1 1997 HCAPLUS

IT **321708-20-7P 321708-25-2P 321708-27-4P**

321708-29-6P 321708-35-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenolic β2-adrenergic receptor agonists)

RN 321708-20-7 HCAPLUS
CN 1,3-Benzenedimethanol, α1,α1'-[trans-1,4-cyclohexanediylbis(iminomethylene)]bis[4-hydroxy- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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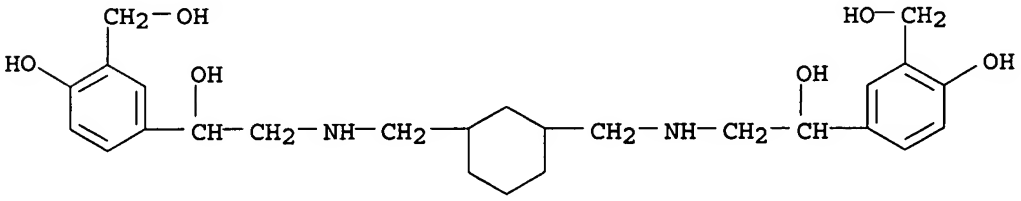
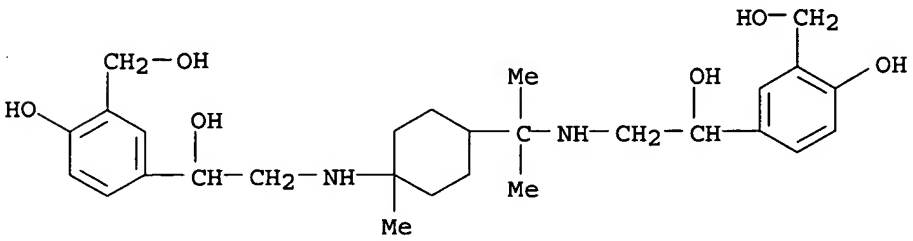


RN 321708-27-4 HCAPLUS
CN 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[1-[4-[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]-4-methylcyclohexyl]-1-methylethyl]amino]methyl]- (9CI) (CA INDEX NAME)



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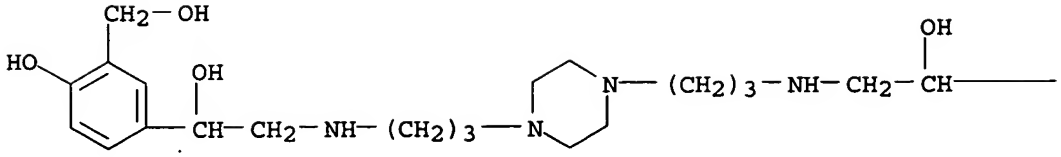

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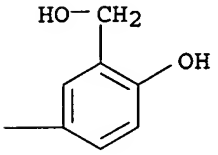
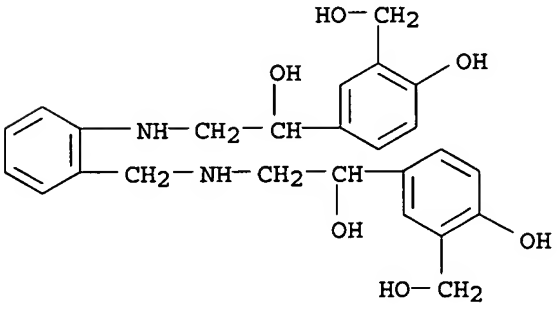


RN 321708-35-4 HCAPLUS
CN 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[2-[[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]methyl]phenyl]amino]methyl]- (9CI) (CA INDEX NAME)



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HIGHEST GRANTED PATENT NUMBER: US6851122
HIGHEST APPLICATION PUBLICATION NUMBER: US2005028237
CA INDEXING IS CURRENT THROUGH 3 Feb 2005 (20050203/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 3 Feb 2005 (20050203/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2004
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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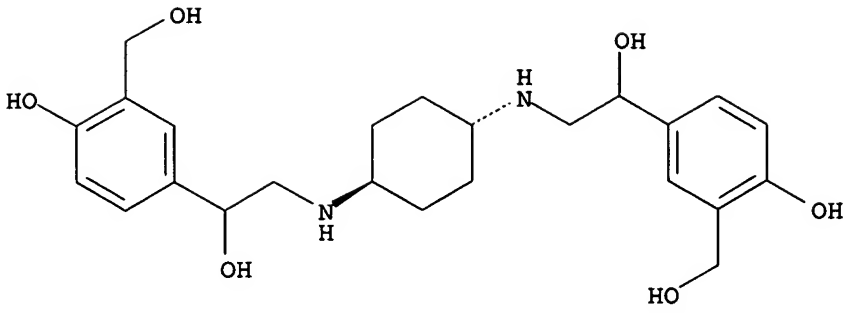
L22 ANSWER 1 OF 1 USPATFULL on STN
AN 2002:106440 USPATFULL
TI Beta2-adrenergic receptor agonists
IN Moran, Edmund J., San Francisco, CA, UNITED STATES
Griffin, John H., Atherton, CA, UNITED STATES
Choi, Seok-Ki, Palo Alto, CA, UNITED STATES
PI US 2002055651 A1 20020509
US 6683115 B2 20040127
AI US 2001-934982 A1 20010821 (9)
RLI Continuation of Ser. No. US 1999-323943, filed on 2 Jun 1999, UNKNOWN
DT Utility
FS APPLICATION
LREP Gerald F. Swiss, BURNS DOANE, SWECKER & MATHIS, L.L.P., P.O.Box 1404, Alexandria, VA, 22313-1404
CLMN Number of Claims: 49
ECL Exemplary Claim: 1
DRWN 10 Drawing Page(s)
LN.CNT 4112
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Disclosed are multibinding compounds which are β2 adrenergic receptor agonists and are useful in the treatment and prevention of respiratory diseases such as asthma, bronchitis. They are also useful in the treatment of nervous system injury and premature labor.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **321708-20-7P**, 1,3-Benzenedimethanol, α1,α1'-[trans-1,4-cyclohexanediylbis(iminomethylene)]bis[4-hydroxy- **321708-25-2P**, 1,3-Benzenedimethanol, α1,α1'-[1,3-cyclohexanediylbis(methyleneiminomethylene)]bis[4-hydroxy- **321708-27-4P**, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[1-[4-[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]-4-methylcyclohexyl]-1-methylethyl]amino]methyl]- **321708-29-6P**, 1,3-Benzenedimethanol, α1,α1'-[1,4-piperazinediylbis(3,1-propanediyliminomethylene)]bis[4-hydroxy- **321708-35-4P**, 1,3-Benzenedimethanol, 4-hydroxy-α1-[[[2-[[[2-hydroxy-2-[4-hydroxy-3-(hydroxymethyl)phenyl]ethyl]amino]methyl]phenyl]amino]methyl]- (preparation of phenolic β2-adrenergic receptor agonists)
RN 321708-20-7 USPATFULL
CN 1,3-Benzenedimethanol, α1,α1'-[trans-1,4-cyclohexanediylbis(iminomethylene)]bis[4-hydroxy- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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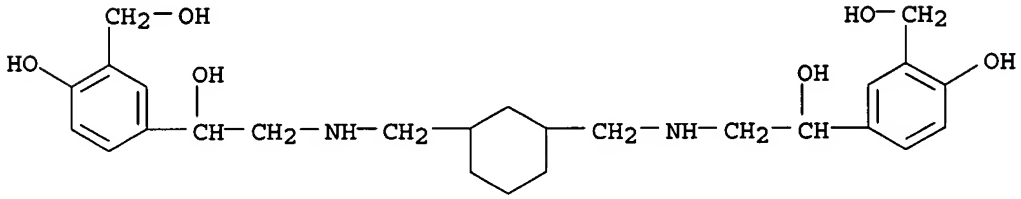

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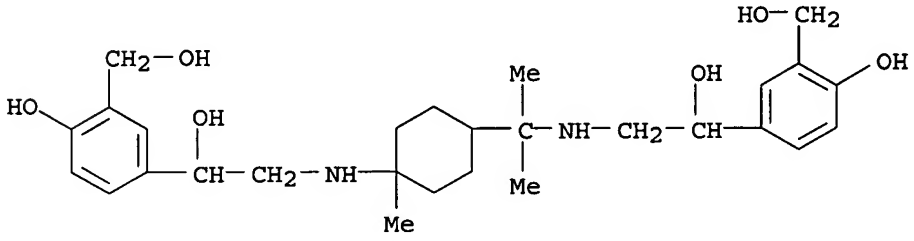

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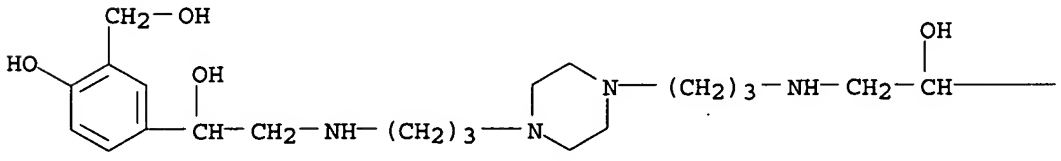

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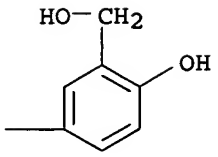

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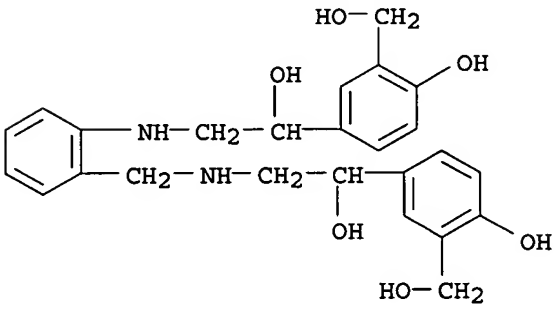

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